STRUCTURAL PREDICTION OF ALLOSTERISM

ABSTRACT

The present invention provides a computer-assisted method for creating and displaying a model of a molecule in which residues that are affected by the binding of a ligand to the molecule are highlighted, making it possible to trace the path of propagation of a binding signal through the molecule. In order to carry out the method, the binding site determinants of the molecule are determined and the binding constant for the ligand is calculated. The states of a conformational ensemble that are binding competent are identified, and the Gibbs energy and probability of each state and the stability constant per residue of the molecule are calculated in the presence and absence of the ligand. Those residues that display a difference in stability constant in the presence vs absence of ligand are those which are affected by the binding of the ligand.